A numerical approach to large deviations in continuous-time

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Abstract.

We present an algorithm to evaluate large deviation functions associated to history-dependent observables. Instead of relying on a time discretisation procedure to approximate the dynamics, we provide a direct continuous-time algorithm valuable for systems with multiple time scales, thus extending the work of Giardinà, Kurchan and Peliti [1].

The procedure is supplemented with a thermodynamic-integration scheme which improves its efficiency. We also show how the method can be used to probe large deviation functions in systems with a dynamical phase transition – revealed in our context through the appearance of a non-analyticity in the large deviation functions.

1. Introduction

The statistical physics of equilibrium systems was first designed to reproduce the macroscopic predictions of thermodynamics, but it was soon realised [2] that it also provides a well-suited frame to describe the fluctuations of physical observables. Such a theory is not available when dealing with non-equilibrium systems or dynamical observables, as one lacks thermodynamics functions such as the free-energy. Over the last decade, there has been a growing interest within the physics community in the theory of large deviation functions [3], as it appeared that they could fill this gap in some cases. For instance, the fluctuations of particle or energy currents Q flowing through a system in the *long time* limit can be obtained from the associated large deviation function $\pi(q = Q/t)$:

$$\mathrm{Prob}(q\,,\,t) \;\sim\; \mathrm{e}^{t\pi(q)} \qquad \text{as} \quad t \to \infty \tag{1}$$

The function $\pi(q)$ is a dynamical analog of the intensive entropy in the microcanonical ensemble and the long time limit plays the role of the thermodynamic limit. In the past few years, a huge amount of effort has been devoted to the study of a strikingly simple symmetry of the large deviation function of the injected power, the so-called fluctuation theorem. The results obtained range from theoretical and numerical studies [4, 5, 6, 7, 8, 9] to experimental applications (see [10] for a glimpse at the literature).

Beyond its symmetries, $\pi(q)$ itself expectedly bears information on the current flowing through the system. For instance, the large deviation function $\pi(q)$ can be fully determined in diffusive systems [11, 12] and its scaling properties differ from those of superdiffusive ones (see [13] for explicit results). In the context of dynamical systems also, large deviation functions associated with more general observables have been introduced [14] and their determinations has received a broad interest [16, 18, 19, 17]. Although the variety of results obtained from these approaches raises hopes for an out-of-equilibrium thermodynamics, the determination of large deviation functions is in general a hard task to achieve and most exact results are confined to simple systems or peculiar models [11, 12, 13]. In more complex cases, we have to rely on numerical evaluations.

However, the very definition of large deviations renders their direct numerical observation almost impossible, as the probability to observe a value of Q/t far from its average typically decreases exponentially with time. Giardinà, Kurchan and Peliti [1] introduced a numerical procedure which overcomes this difficulty for discrete time Markov chains. Nevertheless, most physical processes evolve continuously in time, and one thus has to choose an arbitrary time step dt to discretise the dynamics, balancing between algorithm efficiency and errors arising from the approximation. Typically, dt has to be smaller than any time scale of the system, yet too small a value only increases the simulation duration, since most of the time steps would then be spent in rejected moves. This issue already affects the standard Monte Carlo algorithms, and becomes quite unavoidable when dealing with the computation of large deviation functions. Indeed, even systems featuring a single time scale in the steady state present in general

different time scales in their large deviations, depending on the kind of histories probed, which makes the choice of dt strenuous. A simple example is given by traffic flow models, in which the typical time scale is fixed on average, but vary by a factor equal to the number N of "cars" when comparing jammed histories (where $\mathcal{O}(1)$ cars move) and free flowing histories (where $\mathcal{O}(N)$ cars move).

In the present paper we propose a new procedure where the time discretisation issue is bypassed with a direct continuous-time approach. The outline of the paper is as follows: in section 2, we recall the continuous-time formalism, define the large deviation functions and present the algorithm. In section 3, we study three systems where the continuous-time approach proves useful: the symmetric simple exclusion process, its asymmetric, out of equilibrium counterpart, and the contact process, for which a dynamical phase transition occurs.

2. Formalism and Algorithm

2.1. Continuous time Markov chains

We consider a system described by a finite number of configurations $\{\mathcal{C}\}$, whose evolution is determined by the transition rates $W(\mathcal{C} \to \mathcal{C}')$ between different configurations. The probability $P(\mathcal{C}, t)$ to find the system in $\mathcal{C}$ at time t evolves according to the master equation

$$\partial_t P(\mathcal{C}, t) = \sum_{\mathcal{C}' \neq \mathcal{C}} W(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}', t) \ - r(\mathcal{C}) P(\mathcal{C}, t) \tag{2}$$

where the escape rate $r(\mathcal{C})$ reads

$$r(\mathcal{C}) = \sum_{\mathcal{C}' \neq \mathcal{C}} W(\mathcal{C} \to \mathcal{C}'). \tag{3}$$

Starting from $\mathcal{C}_0$, the system evolves through a succession of configurations $\{\mathcal{C}_k\}_{0 \leq k \leq K}$, jumping from $\mathcal{C}_k$ to $\mathcal{C}_{k+1}$ at time t_k with probability $\frac{W(\mathcal{C}_k \to \mathcal{C}_{k+1})}{r(\mathcal{C}_k)}$ (See Figure 1). Note that contrary to the discrete time case, $\mathcal{C}_k$ and $\mathcal{C}_{k+1}$ are necessarily different. The time elapsed between two consecutive jumps is a random variable: if the system arrives at time t_0 in the configuration $\mathcal{C}_0$, the next move occurs at a time t_1, distributed according to a Poisson law:

$$\rho(t_1 | \mathcal{C}_0, t_0) = r(\mathcal{C}_0) \mathrm{e}^{-(t_1 - t_0) r(\mathcal{C}_0)} \tag{4}$$

2.2. Large deviation functions

Let us consider an observable A extensive in time, which can be written as a sum along a history $\{\mathcal{C}_k\}_{0 \leq k \leq K}$ of elementary contributions $\alpha_{\mathcal{C}_k \mathcal{C}_{k+1}}$:

$$A = \sum_{0 \leq k \leq K-1} \alpha_{\mathcal{C}_k \mathcal{C}_{k+1}} \tag{5}$$

This form is quite generic and most of the commonly studied observables fall in this class. For instance, if A is the overall current of a one dimensional lattice gas, $\alpha_{\mathcal{C}\mathcal{C}'}$

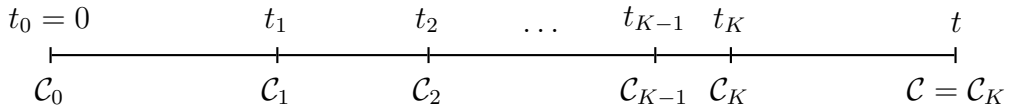

Figure 1. An history of the system between time $t_0 = 0$ and time t.

is the contribution of a single particle jump (See Section 3.1). Moreover, to compute the average of a static observable $\mathcal{O}$ along a history, one simply takes $\alpha_{\mathcal{C}\mathcal{C}'} = \mathcal{O}(\mathcal{C})$ and recover $\langle \mathcal{O} \rangle = \frac{A}{t}$.

In equilibrium statistical mechanics, the difficult task of computing the entropy can be conveniently substituted by the determination of the free energy. Here, instead of working at fixed value of A (microcanonical ensemble) to compute $\pi(A/t)$, one rather introduces a parameter s which fixes the average of A (canonical ensemble). s is intensive in time and plays a role analogous to the inverse temperature in equilibrium thermodynamics. This leads us to introduce the dynamical partition function

$$Z(s,t) = \left\langle \mathrm{e}^{-sta} \right\rangle \sim \mathrm{e}^{t\psi_A(s)} \qquad \text{as} \qquad t \to \infty \tag{6}$$

where the average $\langle \ldots \rangle$ is taken over all histories between 0 and t and $a = A/t$ is intensive in time. The large deviation function $\psi_A(s)$ of $Z(s,t)$ is the Legendre transform of $\pi(a)$

$$\psi_A(s) = \max_a \left[\pi(a) - sa \right]. \tag{7}$$

Under quite general conditions [3], this relation can be inverted and one can get $\pi(a)$ knowing $\psi_A(s)$ through:

$$\pi(a) = \max_s \left[\psi_A(s) + sa \right] \tag{8}$$

To compute $Z(s,t)$, let us first write the master equation obeyed by the joint probability $P(\mathcal{C}, A, t)$ of being in configuration $\mathcal{C}$ with a value A for the observable at time t:

$$\partial_t P(\mathcal{C}, A, t) = \sum_{\mathcal{C}' \neq \mathcal{C}} W(\mathcal{C}' \to \mathcal{C}) P(\mathcal{C}', A - \alpha_{\mathcal{C}'\mathcal{C}}, t) \; - r(\mathcal{C}) P(\mathcal{C}, A, t) \tag{9}$$

The Laplace transform $\hat{P}(\mathcal{C}, s, t) = \sum_A \mathrm{e}^{-sA} P(\mathcal{C}, A, t)$ then evolves with

$$\partial_t \hat{P}(\mathcal{C}, s, t) = \sum_{\mathcal{C}' \neq \mathcal{C}} W_s(\mathcal{C}' \to \mathcal{C}) \hat{P}(\mathcal{C}', s, t) \; - r(\mathcal{C}) \hat{P}(\mathcal{C}, s, t) \tag{10}$$

where the s-modified rates W_s are given by

$$W_s(\mathcal{C}' \to \mathcal{C}) = \mathrm{e}^{-s\,\alpha_{\mathcal{C}'\mathcal{C}}} W(\mathcal{C}' \to \mathcal{C}) \tag{11}$$

From equation (10), one sees that $Z(s,t) = \sum_{\mathcal{C}} \hat{P}(\mathcal{C}, s, t)$ behaves at large time as $\mathrm{e}^{\psi_A(s)t}$ where $\psi_A(s)$ is the largest eigenvalue of a (not probability conserving) evolution operator, which justifies the asymptotic behaviour in (6). The determination of the large deviation functions $\psi_A(s)$ then amounts to the computation of this eigenvalue, which we address in the next section.

2.3. A cloning algorithm

Let us consider the *s-modified* Markov dynamics defined by the rates W_s, whose evolution operator reads

$$(\mathbb{W}_s)_{\mathcal{C}\mathcal{C}'} = W_s(\mathcal{C}' \to \mathcal{C}) - r_s(\mathcal{C})\delta_{\mathcal{C}\mathcal{C}'} \tag{12}$$

where

$$r_s(\mathcal{C}) = \sum_{\mathcal{C}'} W_s(\mathcal{C} \to \mathcal{C}'). \tag{13}$$

The evolution of $\hat{P}(\mathcal{C}, s, t)$ can be written as

$$\partial_t \hat{P}(\mathcal{C}, s, t) = \sum_{\mathcal{C}'} (\mathbb{W}_s)_{\mathcal{C}\mathcal{C}'}\, \hat{P}(\mathcal{C}', s, t) + [r_s(\mathcal{C}) - r(\mathcal{C})]\hat{P}(\mathcal{C}, s, t) \tag{14}$$

The corresponding dynamics alternates changes of configuration determined by the s-modified rates and exponential evolution of the "non-conserved probability" $\hat{P}(\mathcal{C}, s, t)$ with rate $r_s(\mathcal{C}) - r(\mathcal{C})$ (corresponding respectively to the first and second term of the r.h.s of (14)). More details are given in Appendix A. The evolution of $Z(s,t) = \sum_{\mathcal{C}} \hat{P}(\mathcal{C}, s, t)$ is consequently represented by a population dynamics a la Diffusion Monte Carlo [20]. Let us consider $\mathcal{N}_0$ clones of the system evolving in parallel with the s modified dynamics. At any change of configuration of any clone c_α,

(1) c_α jumps from its configuration $\mathcal{C}$ to another configuration $\mathcal{C}'$ with probability $W_s(\mathcal{C} \to \mathcal{C}')/r_s(\mathcal{C})$.

(2) The time interval Δt until the next jump of c_α is chosen from the Poisson law (4) of parameter $r_s(\mathcal{C}')$.

(3) The clone c_α is either cloned or pruned with a rate $\mathcal{Y}(\mathcal{C}') = \mathrm{e}^{\Delta t(r_s(\mathcal{C}') - r(\mathcal{C}'))}$
   a) One computes $y = \lfloor \mathcal{Y}(\mathcal{C}') + \varepsilon \rfloor$ where ε is uniformly distributed on $[0, 1]$.
   b) If $y = 0$, the copy c_α is erased.
   c) If $y > 1$, we make $y - 1$ new copies of c_α

Such a cloning procedure modifies the total number of clones by a factor $X = \frac{\mathcal{N}+y-1}{\mathcal{N}}$, which represents the exponential evolution of $\hat{P}(\mathcal{C}', s, t)$. Finally, $Z(s,t)$ is simply given by the increase of the population:

$$Z(s,t) = \frac{\mathcal{N}(t)}{\mathcal{N}_0} \tag{15}$$

However, such an algorithm may result in an exponential growth or a complete decay of the clones and we consequently add a 4^{th} step to maintain their number constant:

(4) If $y = 0$, one clone $c_\beta \neq c_\alpha$ is chosen at random and copied, while if $y > 1$, $y - 1$ clones are chosen uniformly among the $N + y - 1$ clones and erased. To reconstruct $Z(s,t)$, we keep track of all X factors

The large deviation function $\psi_A(s)$ is then recovered from the long time behaviour of the product of the cloning factors:

$$\frac{1}{t} \ln X_1 \dots X_{\mathcal{K}} = \frac{1}{t} \ln \left\langle \mathrm{e}^{-sta} \right\rangle \sim \psi_A(s) \qquad \text{as} \qquad t \to \infty \tag{16}$$

where $\mathcal{K}$ is the total number of configuration changes among all the histories between 0 and t.

Another interpretation of such a population dynamics has been discussed by Grassberger in [15] for the discrete time case and we shall present it shortly. A formal integration of (14) leads to

$$\left\langle \mathrm{e}^{-sta} \right\rangle = \left\langle \mathrm{e}^{\int_0^t r_s(\mathcal{C}(t))-r(\mathcal{C}(t))dt} \right\rangle_s \tag{17}$$

where the average $\langle \ldots \rangle_s$ is taken over all trajectories from 0 to t of the s-modified dynamics. The change of rates $W \to W_s$ can be seen a sequential importance sampling, which favours histories relevant for the computation of $Z(s,t)$. The exponential within the r.h.s. of (17) can be seen as a weight over trajectories. Along the simulation, clones with a high weight w_H are replaced by w_H clones with a weight 1, while clones with low weight w_L are either deleted with probability $1-w_L$ or given a weight 1 with probability w_L. This is very close to the cloning strategy followed at step (3).

Let us finally note that one can define a new measure over the space of trajectories, such that the average of an observable $\mathcal{B}$ reads

$$\overline{\mathcal{B}^s} = \frac{\langle \mathcal{B}\mathrm{e}^{-sta} \rangle}{\langle \mathrm{e}^{-sta} \rangle} \tag{18}$$

This is the measure observed in the simulations with a fixed number of clones, as one can see that the denominator is nothing but the unconstrained population at time t.

2.4. Thermodynamic integration

The direct computation of $\psi_A(s)$ is in general quite noisy, because of the finiteness of the clones population. One can alternatively compute $\psi'_A(s)$ and then integrate it. From the definition of ψ_A :

$$\psi_A(s) = \frac{1}{t} \ln \left\langle \mathrm{e}^{-sta} \right\rangle \tag{19}$$

one gets by derivation

$$\psi'_A(s) = -\frac{\langle a\mathrm{e}^{-sta} \rangle}{\langle \mathrm{e}^{-sta} \rangle} = -\overline{a^s} \tag{20}$$

which is nothing but the average value of a within the population of clones. Finally,

$$\psi_A(s) = -\int_0^s \overline{a^r} dr \tag{21}$$

Thanks to the integration, the noise is smoothed out.

3. Three examples

3.1. The Symmetric Exclusion Process (SEP)

We now apply the algorithm to the large deviations of the total current Q in the Symmetric Exclusion Process [21] with closed boundary conditions. The system is

composed of N particles diffusing on a one-dimensional lattice of size L. Each particle can jump with rate 1 to any neighbouring site, provided it is empty. The total current Q increases or decreases by 1 at every move, depending on the direction of the jump. Using the notation (5), $\alpha_{CC'} = 1$ or -1 when a particle moves to its right or to its left, respectively.

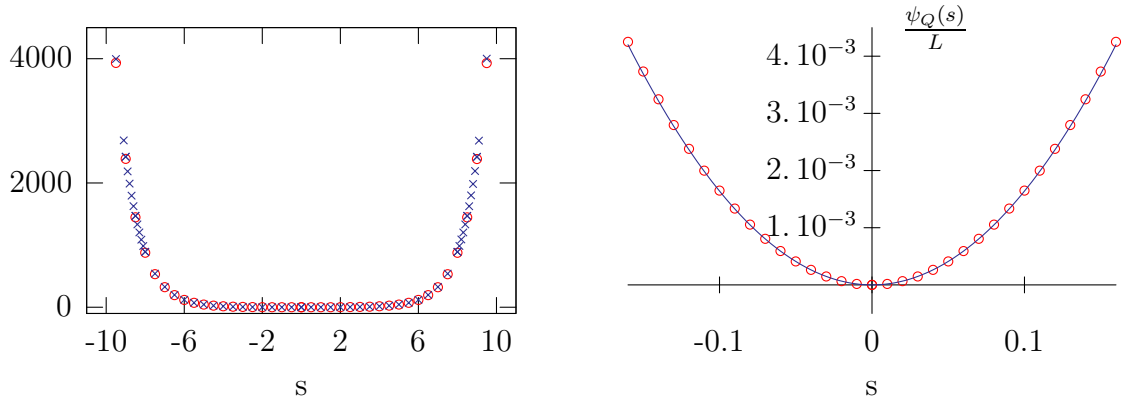

Figure 2. Numerical evaluation of $\frac{1}{L}\psi_Q(s)$ for the Simple Exclusion Process ($N = 200$, $L = 400$). (a: **Left**) Comparison between direct numerical measurement (blue crosses) and result from thermodynamic integration (red circles).
(b: **Right**) Comparison between numerical results (red circles) and analytical prediction (22) valid for small s (blue line).

As in other exclusion processes [9, 13], the large deviation function $\psi_Q(s)$ is extensive in the system size and we rather study the rescaled large deviation function $\frac{1}{L}\psi_Q(s)$ in the thermodynamic limit (N and L are large, the density $\rho = N/L$ being fixed). Though on average the total current is zero (the moves are symmetric), the variance is finite and $\psi_Q(s)$ reads for small s [11, 21]

$$\frac{1}{L}\psi_Q(s) = \rho(1-\rho)s^2 + \mathcal{O}(Ls^4) \tag{22}$$

In this regime, the fluctuations are Gaussian and our algorithm yields results in perfect agreement with the expansion (22) (see Figure 2b). For larger values of s, we lack an analytic expression for $\psi_Q(s)$ but the algorithm still applies successfully. We found non-Gaussian fluctuations (Figure 2a), which correspond to very large deviations of the current.

The direct measurement of $\psi_Q(s)$ is also compared with the results obtained from thermodynamic integration (Figure 2a). Both evaluations coincide within numerical accuracy, though the latter requires duration more than one order of magnitude smaller to converge.

3.2. The Asymmetric Simple Exclusion Process (ASEP)

We now consider the large deviations of the total current Q in a non-equilibrium system, the Asymmetric Simple Exclusion Process [21] with closed boundary conditions. The

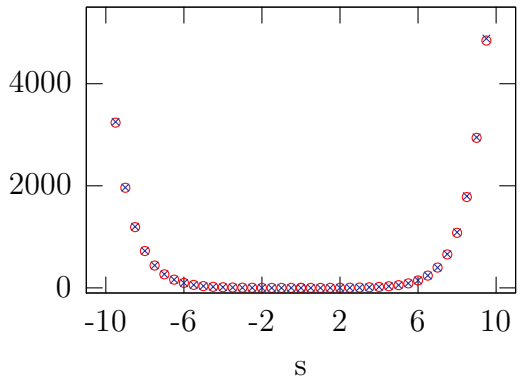

Figure 3. Plot of the large deviation function $\frac{1}{L}\psi_Q(s)$ of the Asymmetric Simple Exclusion Process, for $L = 400$ sites and $N = 200$ particles. The jump rates are $p = 1.2$ and $q = 0.8$, whence $E \simeq -0.2$. Blue crosses and red circles correspond to direct computation and thermodynamic integration respectively. The asymmetry appears when comparing the extreme points $s = \pm 9.5$.

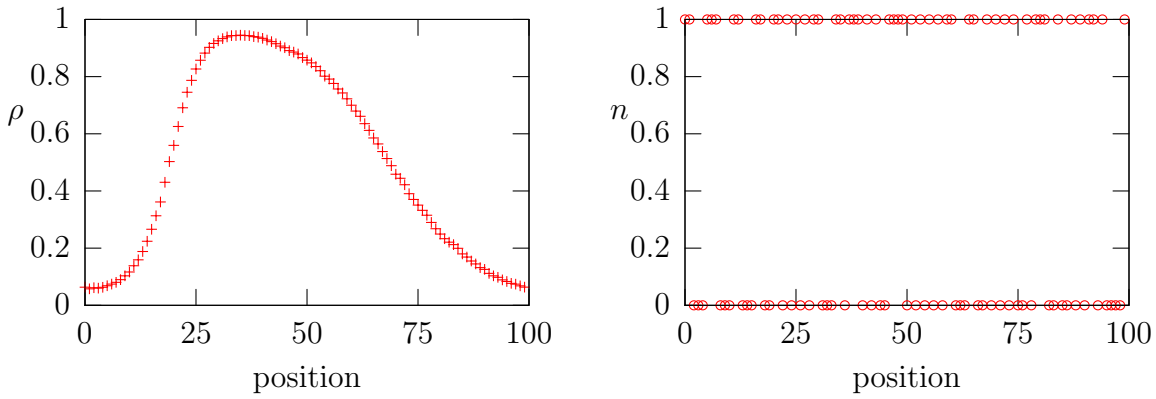

Figure 4. (a: **Left**) Average profile ρ for $s = 0.3$. To minimise the overall current, the system develops an asymmetric shock, where only the front particles can jump easily. (b: **Right**) A typical configuration for $|s| \gg E$. The particles are distributed almost uniformly.

system is composed of N particles diffusing on a one-dimensional lattice of size L. Each particle can jump with rate p to its left and q to its right, provided the arrival site is empty. The total current Q is defined as in the previous section. For $p \neq q$, a non-zero steady current flows through the system. We report in Figure 3 the large deviation function $\psi_Q(s)$. One notes the symmetry around $E = \frac{1}{2}\ln\frac{q}{p}$, guaranteed by the fluctuation theorem. The histories which contribute to $\psi_Q(s)$ around $s \approx E$ ($Q \approx 0$) clearly display shocks (Figure 4**a**) while a large current ($|s| \gg E$) is provided by uniform profiles (Figure 4**b**).

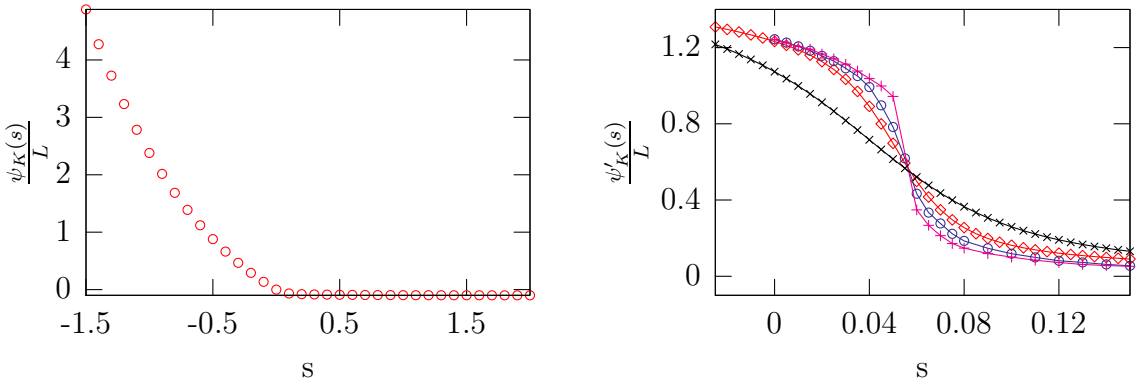

Figure 5. (a: **Left**) Plot of the large deviation function $\frac{1}{L}\psi_K(s)$ associated to the number of events K in the Contact Process in a field ($L = 120$ sites) (b: **Right**) The dynamical phase transition occurs at $s_c \sim 0.057$. This is exemplified by plotting $\psi'_K(s) = \frac{1}{t}\langle K\rangle_s$ for different system sizes ($L = 4$ in black, 8 in red, 15 in blue and 50 in magenta)

3.3. The Contact Process (CP)

We now turn our attention to the Contact Process [23] in one dimension. The model is defined on a lattice of L sites with periodic boundary conditions. Each site i is either empty ($n_i = 0$) or occupied by a particle ($n_i = 1$). The dynamics is defined as follows: particles annihilate with rate 1, while empty sites i get occupied with rate

$$W(n_i = 0 \to n_i = 1) = \lambda(n_{i-1} + n_{i+1}) + h \tag{23}$$

where λ and h are positive constants. Note the presence of a spontaneous rate of creation h. When $h = 0$, the systems always reaches an absorbing empty state in finite size [24, 25], while the steady state is active for $\lambda > 1$ in the thermodynamic limit.

On the contrary, the addition of a small field h leads to an active equilibrium state for all λ. In the mean field version, the equilibrium dynamics is still influenced by the presence of an inactive state. This can be seen through the study of the large deviations of the number of events K, a quantity which simply counts the number of configuration changes during an history of the system. It was proved that $\frac{1}{L}\psi_K(s)$ is non-analytic at a critical value s_c, which goes to zero with h. As pointed out in section 2.2 the large deviation function $\psi_K(s)$ plays the role of a dynamical free energy, whose non-analyticities are synonymous of dynamical phase transitions. In physical terms, this corresponds to the existence of two distinct classes of histories [19]: the active phase dominates the steady state, while large deviations corresponding to $s > s_c$ are dominated by inactive histories. For $s = s_c$, the two phases coexist in a first-order fashion. The question whether this transition is still present in finite dimension is still open.

Using our algorithm, we obtain evidence that this is indeed the case in dimension 1. In Figure 5a, we plot the function $\psi_K(s)$ for a large system size and for values of the parameters $\lambda = 3.5$, $h = 0.1$. The two branches of the function correspond to

the two dynamical phases mentioned above. As in the mean field version, the non-analycity appears as a jump in the first derivative of $\frac{1}{L}\psi_K(s)$ in the thermodynamic limit. Using the relation $\psi'_K(s) = -\frac{1}{t}\overline{K^s}$ (see section 2.4), we can study the finite size scaling of $\frac{1}{L}\psi'_K(s)$ (Figure 5). The results support the presence of a phase transition at $s_c \sim 0.057$. Around s_c, the dynamics presents a superposition of "more active" and "less active" histories, for which the continuous-time approach is particularly helpful.

4. Conclusions

We have presented a simple algorithm to evaluate large deviation functions in continuous-time Markov chains without relying on any time discretisation. We have shown on specific examples that the method can be used successfully in systems where the presence of different time scales renders the discrete-time approach difficult.

In the context of quantum simulations, an approach to continuous-time versions of Diffusion Monte Carlo was proposed by Syljuåsen [26], using a continuous formalism but a discrete time implementation. One can expect that the algorithm we have introduced could also be interesting in such context.

Acknowledgments

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Appendix A.

An explicit formula for $Z(s,t)$ can be written as the sum over $\mathcal{C}$ of the solution of (14):

$$Z(s,t) = \sum_{K\geq 0}\sum_{\mathcal{C}_1,\dots,\mathcal{C}_{K-1},\mathcal{C}} \int_0^t d\mu^s_{t_K}\int_0^{t_K} d\mu^s_{t_{K-1}}\dots\int_0^{t_2} d\mu^s_{t_1} \mathrm{e}^{-(t-t_K)r_s(\mathcal{C})} \qquad \text{(A.1)}$$
$$\mathcal{Y}(\mathcal{C}_0)^{t_1-t_0}\frac{W_s(\mathcal{C}_0\to\mathcal{C}_1)}{r_s(\mathcal{C}_0)}\dots\mathcal{Y}(\mathcal{C}_{K-1})^{t_K-t_{K-1}}\frac{W_s(\mathcal{C}_{K-1}\to\mathcal{C})}{r_s(\mathcal{C}_{K-1})}\mathcal{Y}(\mathcal{C})^{t-t_K}$$

where

$$r_s(\mathcal{C}) = \sum_{\mathcal{C}'\neq\mathcal{C}} W_s(\mathcal{C}\to\mathcal{C}') \qquad \text{(A.2)}$$

is the escape rate from the configuration $\mathcal{C}$ in the s-modified dynamics,

$$d\mu^s_{t_k} = dt_k\, r_s(\mathcal{C}_k)\exp[-(t_k - t_{k-1})r_s(\mathcal{C}_k)] \qquad \text{(A.3)}$$

represents the probability of the time intervals between jumps, and

$$\mathcal{Y}(\mathcal{C}_k)^{t_{k+1}-t_k} = \mathrm{e}^{(t_{k+1}-t_k)(r_s(\mathcal{C}_k)-r(\mathcal{C}_k))} \tag{A.4}$$

is the exponential increase of $\hat{P}$ between t_k and t_{k+1}. We can read in this formula the direct expression of the cloning factors used at the step (3) of the algorithm.

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